Adhesive Hard-Sphere Yukawa Model for Colloidal Gels

L. Lue and C.D. Muzny
Physical and Chemical Properties Division
Chemical Science and Technology Laboratory
National Institute of Standards and Technology
325 Broadway
Boulder, CO 80303-3328 U.S.A.

We present a microscopically based theory for the behavior of colloidal gels. The interactions between the colloidal particles $u(r)$ is modeled using the adhesive hard-sphere Yukawa potential:

$$\frac{u(r)}{k_B T} = +\infty \qquad \text{for r} < \sigma$$

$$\frac{u(r)}{k_B T} = -\frac{G}{\sigma}\delta(r-\sigma) \quad + \quad \frac{K}{r}e^{-\kappa T} \quad \text{for r} \geq \sigma$$

where k_B is the Boltzmann constant, T is the absolute temperature of the system, σ is the diameter of the colloidal particles, G is a parameter describing short-range attractive interactions due to chemical bonding between colloidal particles, van der Waals interactions, etc., K is related to the surface charge of the colloidal particles, κ is the inverse screening length in the system. Unlike many previous theoretical approaches to gelation (e.g., computer simulation), the parameters of this interaction model can be directly related to the properties of the system such as the solution ionic strength, etc. This model potential yields an analytical structure factor [1] which quantitatively reproduces experimental neutron scattering curves with reasonable parameter values.

From mode coupling theory [2], we calculate the dynamical properties of the system. In particular, we predict the decay of the normalized density-density autocorrelation function $\phi_q(t)$ at various system conditions. In addition, from parameter values where the asymptotic long-time limit of $\phi_q(t)$ is nonzero, we construct a phase diagram of where the colloid system forms a gel (i.e., the ergodicity of the system is broken.).

[1] M. Yasutomi and M. Ginoza, *Molec. Phys*. **89**, 1755 (1996).
[2] H. Z. Cummins, *J. Phys: Condens. Matter* **11**, A95 (1999).